Robert Havlin - 10.544899

FILE 'REGISTRY' ENTERED AT 10:27:10 ON 26 APR 2007
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 25 APR 2007 HIGHEST RN 932710-95-7
DICTIONARY FILE UPDATES: 25 APR 2007 HIGHEST RN 932710-95-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
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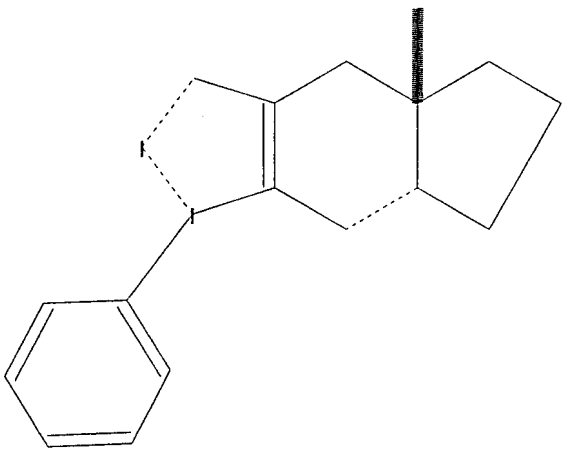
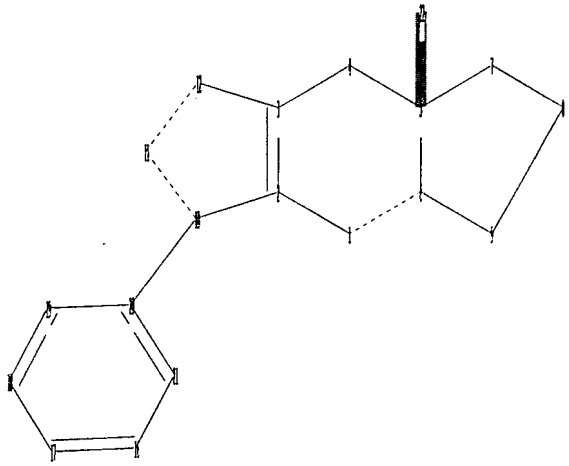
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10.544899\elected group.str





chain nodes :
22
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 16 17 18 19 20 21
chain bonds :
5-22 10-20
ring bonds :
1-2 1-6 2-3 2-10 3-4 3-12 4-5 5-6 5-7 6-9 7-8 8-9 10-11 11-12 16-17 16-21 17-18
18-19 19-20 20-21
exact/norm bonds :
1-6 8-9 10-11 10-20 11-12
exact bonds :
1-2 2-3 2-10 3-4 3-12 4-5 5-6 5-7 5-22 6-9 7-8
normalized bonds :
16-17 16-21 17-18 18-19 19-20 20-21
isolated ring systems :
containing 1 :

G1:C,N

Match level :

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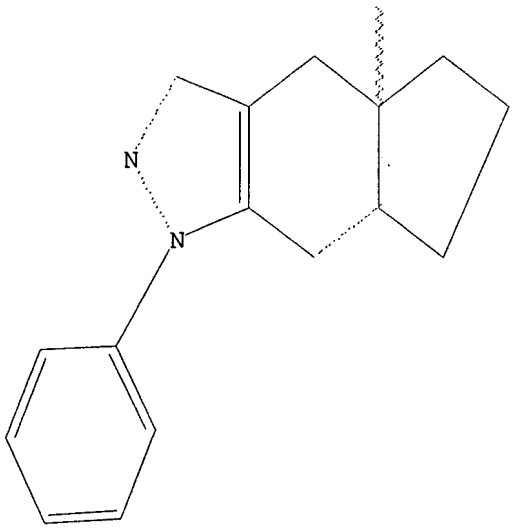
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 C,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
SAMPLE SEARCH INITIATED 10:28:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 110 TO ITERATE

100.0% PROCESSED 110 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

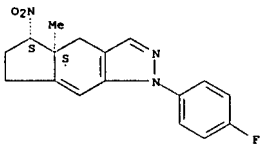
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1571 TO 2829
PROJECTED ANSWERS: 56 TO 504

L2 14 SEA SSS SAM L1

=> d scan

L2 14 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopent[f]indazole, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-5-nitro-, (4aS,5S)- (9CI)
MF C17 H16 F N3 O2

Absolute stereochemistry.

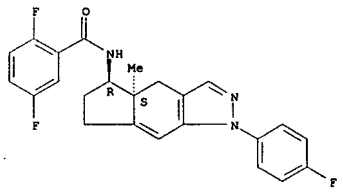


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 14 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzamide, 2,5-difluoro-N-[(4aS,5R)-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methylcyclopent[f]indazol-5-yl]- (9CI)
MF C24 H20 F3 N3 O

Absolute stereochemistry.

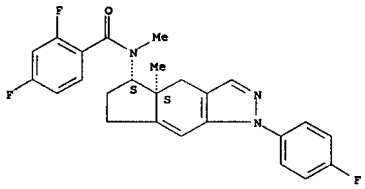


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L2 14 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Benzamide, 2,4-difluoro-N-[(4aS,5S)-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methylcyclopent[f]indazol-5-yl]-N-methyl- (9CI)
MF C25 H22 F3 N3 O

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

Robert Havlin - 10.544899

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=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.90       1.11

FILE 'HCAPLUS' ENTERED AT 10:28:33 ON 26 APR 2007
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 26 Apr 2007  VOL 146 ISS 18
FILE LAST UPDATED: 25 Apr 2007  (20070425/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> s l2
L3            3 L2

=> d ibib abs hitstr tot
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L3 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:927012 HCAPLUS
DOCUMENT NUMBER: 141:395547
TITLE: Preparation of selective spirocyclic glucocorticoid receptor modulators
INVENTOR(S): Ali, Amjad; Balkovec, James M.; Beresis, Richard; Colletti, Steven L.; Graham, Donald W.; Patel, Gool F.; Smith, Cameron J.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 201 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004093805	A2	20041104	WO 2004-US12102	20040419
WO 2004093805	A3	20051208		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004232301	A1	20041104	AU 2004-232301	20040419
CA 2522946	A1	20041104	CA 2004-2522946	20040419
EP 1617806	A2	20060125	EP 2004-760029	20040419
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1809347	A	20060726	CN 2004-80017051	20040419
JP 2006524251	T	20061026	JP 2006-513140	20040419
US 2006217563	A1	20060928	US 2005-551933	20051004

PRIORITY APPLN. INFO.: US 2003-464784P P 20030423
WO 2004-US12102 W 20040419

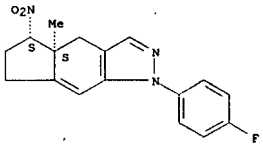
OTHER SOURCE(S): MARPAT 141:395547
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Ring A = carbocyclyl or heterocyclyl; m = 0-3; n = 0-2; R1 = (un)substituted-alkyl, -alkenyl, -alkynyl, -cycloalkyl, etc.; R2 and R3 independently = H, halo, alkyl, aryl, etc.; R4 = OH, CO2H, (un)substituted-alkyl, -Ph, etc.] , as well as their pharmaceutically acceptable salts or hydrates thereof, are prepared and disclosed as selective glucocorticoid receptor ligands for treating a variety of autoimmune and inflammatory diseases or conditions. Thus, e.g., II was prepared via spirocyclization of III (preparation given) with Et α-bromomethyl acrylate. In human glucocorticoid receptor assays, I demonstrated a range of GR affinity with IC50 values between 10 μM and 1 nM. Pharmaceutical compns. and methods of use are also included.
IT 786706-88-5P 786706-89-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

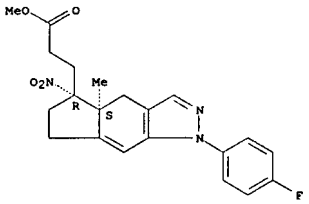
L3 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(prepn. of pyrazoles bearing annulated spirocyclic hydronaphthalene derivs. as glucocorticoid receptor modulators)
RN 786706-88-5 HCAPLUS
CN Cyclopent[f]indazole, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-5-nitro-, (4aS,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 786706-89-6 HCAPLUS
CN Cyclopent[f]indazole-5-propanoic acid, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-5-nitro-, methyl ester, (4aS,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

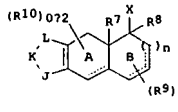


L3 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:740124 HCAPLUS
DOCUMENT NUMBER: 141:260743
TITLE: Preparation of cyclopent[f]indazole and benz[f]indazole derivatives selective non-steroidal glucocorticoid receptor modulators
INVENTOR(S): Ali, Amjad; Beresis, Richard; Colletti, Steven L.; Graham, Donald W.; Tata, James R.; Thompson, Christopher F.
PATENT ASSIGNEE(S): Merck & Co. Inc., USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004075840	A2	20040910	WO 2004-US5199	20040220
WO 2004075840	A3	20050203		
WO 2004075840	A9	20050804		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004216182	A1	20040910	AU 2004-216182	20040220
CA 2516684	A1	20040910	CA 2004-2516684	20040220
EP 1599201	A2	20051130	EP 2004-713398	20040220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006518752	T	20060817	JP 2006-503780	20040220
US 2006074120	A1	20060406	US 2005-544899	20050808

PRIORITY APPLN. INFO.: US 2003-450811P P 20030225
WO 2004-US5199 W 20040220

OTHER SOURCE(S): MARPAT 141:260743
GI



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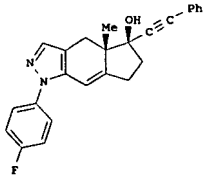
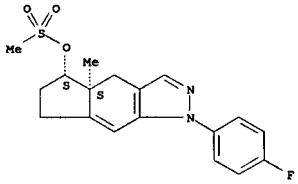


II

L3 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Title compds. represented by the formula I [wherein J = NR1, CR1R2; K = NR3, CR3R4; L = NR5, CR5R6; X = hydroxy, alkoxy, carbamoyl, etc.; R1-R6 = independently H, halo, (cyclo)alkyl, etc.; R7 = H, hydroxy, alkoxy, aryl, etc.; R8 = (cyclo)alkyl, alkenyl, alkynyl, etc.; R9, R10 = independently halo, hydroxy, alkyl, alkenyl, alkoxy; n = 0-2; and pharmaceutically acceptable salts or hydrates thereof] were prepared as selective non-steroidal glucocorticoid receptor modulators. For example, II was given in a multi-steps synthesis starting from 1-(4-fluorophenyl)-4,4a,6,7-tetrahydro-4a-methyl-cyclopent[f]indazol-5(1H)-one reacting with phenylethynylmagnesium bromide. I showed affinity of glucocorticoid receptor with IC50 values between 10 μM and 1 nM. Thus, I and their pharmaceutical compns. are useful for the treatment of a variety of autoimmune and inflammatory diseases or conditions.
IT 754237-88-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of cyclopent[f]indazol-5-yl and benz[f]indazol-5-yl derivs. as selective non-steroidal glucocorticoid receptor modulators)
RN 754237-88-2 HCAPLUS
CN Cyclopent[f]indazol-5-ol, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-, methanesulfonate (ester), (4aS,5S)- (9CI) (CA INDEX NAME)

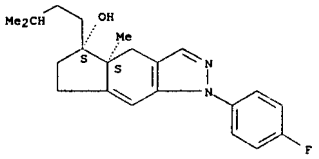
Absolute stereochemistry.



IT 754236-00-5P 754236-04-9P 754236-65-2P
754236-75-4P 754237-30-4P 754237-65-5P
754238-00-1P 754238-30-7P 754238-35-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopent[f]indazol-5-yl and benz[f]indazol-5-yl derivs. as selective non-steroidal glucocorticoid receptor modulators)
RN 754236-00-5 HCAPLUS
CN Cyclopent[f]indazol-5-ol, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-5-(3-methylbutyl)-, (4aS,5S)- (9CI) (CA INDEX NAME)

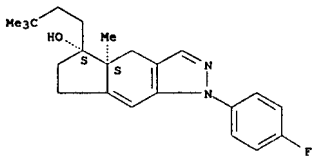
Absolute stereochemistry.

L3 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



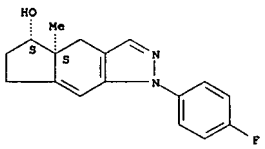
RN 754236-04-9 HCAPLUS
CN Cyclopent[f]indazol-5-ol, 5-(3,3-dimethylbutyl)-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-, (4aS,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 754236-65-2 HCAPLUS
CN Cyclopent[f]indazol-5-ol, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-, (4aS,5S)- (9CI) (CA INDEX NAME)

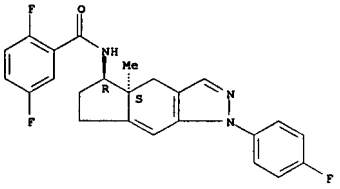
Absolute stereochemistry.



RN 754236-75-4 HCAPLUS
CN Cyclopent[f]indazole, 5-[2-(3-chlorophenyl)ethyl]-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-5-propoxy-, (4aS,5S)- (9CI) (CA INDEX NAME)

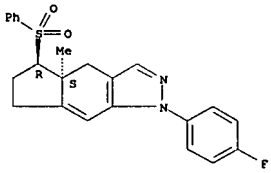
Absolute stereochemistry.

L3 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



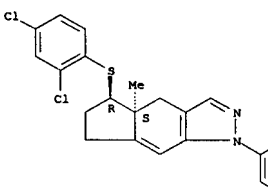
RN 754238-00-1 HCAPLUS
CN Benzamide, 2,5-difluoro-N-[(4aS,5R)-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methylcyclopent[f]indazol-5-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 754238-30-7 HCAPLUS
CN Cyclopent[f]indazole, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-5-(phenylsulfonyl)-, (4aS,5R)- (9CI) (CA INDEX NAME)

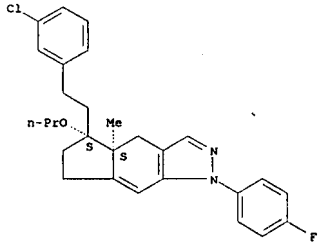
Absolute stereochemistry.



RN 754238-35-2 HCAPLUS
CN Cyclopent[f]indazole, 5-[(2,4-dichlorophenyl)thio]-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-, (4aS,5R)- (9CI) (CA INDEX NAME)

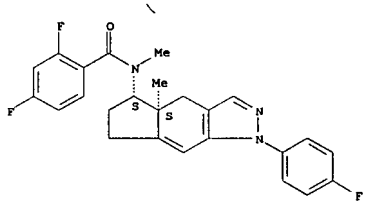
Absolute stereochemistry.

L3 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



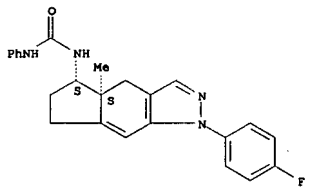
RN 754237-30-4 HCAPLUS
CN Benzamide, 2,4-difluoro-N-[(4aS,5S)-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methylcyclopent[f]indazol-5-yl]-N-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 754237-65-5 HCAPLUS
CN Urea, N-[(4aS,5S)-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methylcyclopent[f]indazol-5-yl]-N'-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

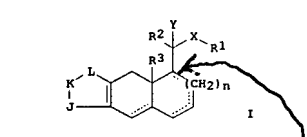


L3 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:836773 HCAPLUS
DOCUMENT NUMBER: 139:323524
TITLE: Preparation of 1H-Benzo[f]indazol-5-yl derivatives as selective glucocorticoid receptor modulators
INVENTOR(S): Ali, Amjad; Balkovec, James M.; Graham, Donald W.; Thompson, Christopher F.; Quraishi, Nazia
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 233 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003086294	A2	20031023	WO 2003-US10867	20030408
WO 2003086294	A3	20040715		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2481320	A1	20031023	CA 2003-2481320	20030408
AU 2003221706	A1	20031027	AU 2003-221706	20030408
EP 1496892	A2	20050119	EP 2003-718285	20030408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005528385	T	20050922	JP 2003-583321	20030408
US 2005256315	A1	20051117	US 2005-508897	20050428
PRIORITY APPLN. INFO.:			US 2002-371948P	P 20020411
			WO 2003-US10867	W 20030408

OTHER SOURCE(S): MARPAT 139:323524
GI



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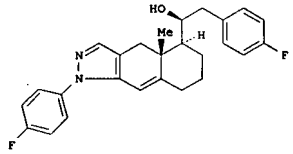


II

Distinguished by lack of -O,-S,-N at this position (n=0)

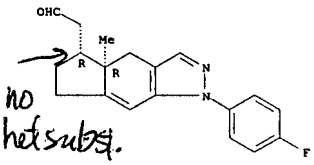
AB Benzindazoles I [n = 0-2; J, K, L = (un)substituted CH2, NH; X = bond, CO, (un)substituted NH, NHCO, 1,1-cyclopropanediyl; R1, R2 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, aryl, aralkyl, heterocyclic, aryloxy, aroyloxy, OH; R3 = H, (un)substituted OH, alkyl, aryl, aralkyl; Y = H, (un)substituted OH, SH, S(O)H, SO2H, CH2, NH2, SO2NH2, CO2H, NO2, acyl, CN, halogen; and the carbocyclic rings may be further substituted] were prepared for use as selective glucocorticoid receptor ligands for treating a variety of autoimmune and inflammatory diseases or conditions (no data). Thus, Wieland-Miescher ketone was ketalized, hydroxymethylenated, cyclized with 4-FC6H4NHNH2, deketalized, treated with Ph3P+CH2OMe Cl-, and subjected to Grignard reaction with 4-FC6H4MgCl to give the benzindazole II.

IT 614763-27-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1H-benzo[f]indazol-5-yl derivs. as selective glucocorticoid receptor modulators)

RN 614763-27-8 HCAPLUS

CN Cyclopent[f]indazole-5-acetaldehyde, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-, (4aR,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



no het subst.

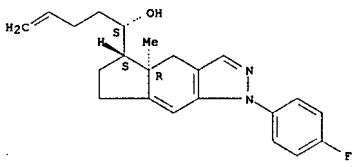
IT 614761-89-6P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1H-benzo[f]indazol-5-yl derivs. as selective glucocorticoid receptor modulators)

RN 614761-89-6 HCAPLUS

CN Cyclopent[f]indazole-5-methanol, α-3-butenyl-1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-, (αS,4aR,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L3 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



Robert Havlin - 10.544899

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                    34.01      35.12

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                    -2.34      -2.34

FILE 'REGISTRY' ENTERED AT 10:32:56 ON 26 APR 2007
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provided by InfoChem.

STRUCTURE FILE UPDATES:   25 APR 2007  HIGHEST RN 932710-95-7
DICTIONARY FILE UPDATES:  25 APR 2007  HIGHEST RN 932710-95-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> s l1 sss full
FULL SEARCH INITIATED 10:33:05 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     2196 TO ITERATE

100.0% PROCESSED     2196 ITERATIONS                          272 ANSWERS
SEARCH TIME: 00.00.01

L4          272 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   172.10     207.22

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -2.34

FILE 'HCAPLUS' ENTERED AT 10:33:15 ON 26 APR 2007
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FILE COVERS 1907 - 26 Apr 2007 VOL 146 ISS 18
FILE LAST UPDATED: 25 Apr 2007 (20070425/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

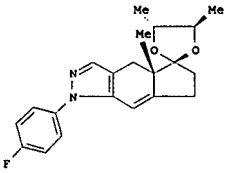
=> s l4
L5 4 L4

=> s l5 not l3
L6 1 L5 NOT L3

=> d ibib abs hitstr

L6 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:461153 HCAPLUS
DOCUMENT NUMBER: 143:125827
TITLE: Novel ketal ligands for the glucocorticoid receptor: in vitro and in vivo activity
AUTHOR(S): Smith, Cameron J.; Ali, Amjad; Balkovec, James M.; Graham, Donald W.; Hammond, Milton L.; Patel, Gool F.; Rouen, Gregory P.; Smith, Scott K.; Tata, James R.; Einstein, Monica; Ge, Lan; Harris, Georgianna S.; Kelly, Theresa M.; Mazur, Paul; Thompson, Chris M.; Wang, Chuanlin F.; Williamson, Joanne M.; Miller, Douglas K.; Pandit, Shilpa; Santoro, Joseph C.; Sitlani, Ayesha; Yamin, Ting-ting D.; O'Neill, Edward A.; Zaller, Dennis M.; Carballo-Jane, Ester; Forrest, Michael J.; Luell, Silvi
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(11), 2926-2931
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:125827
GI



I

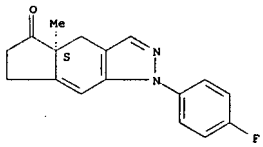
AB A novel series of selective ligands for the human glucocorticoid receptor is described. Structure-activity studies focused on variation of B-ring size, ketal ring size, and ketal substitution. These analogs were found to be potent and selective ligands for GR and have partial agonist profiles in functional assays for transactivation (TAT, GS) and transrepression (IL-6). Of these compds., three were evaluated further in a mouse LPS-induced TNF-α secretion model. Compound (I) had an ED50 of 14.1 mg/kg compared with 0.5 mg/kg for prednisolone in the same assay.

IT 614763-02-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel ketal ligands for glucocorticoid receptor and in vitro and in vivo activity)

RN 614763-02-9 HCAPLUS
CN Cyclopent[f]indazol-5(1H)-one, 1-(4-fluorophenyl)-4,4a,6,7-tetrahydro-4a-methyl-, (4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L6 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	10.47	217.69

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.78	-3.12

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:34:35 ON 26 APR 2007

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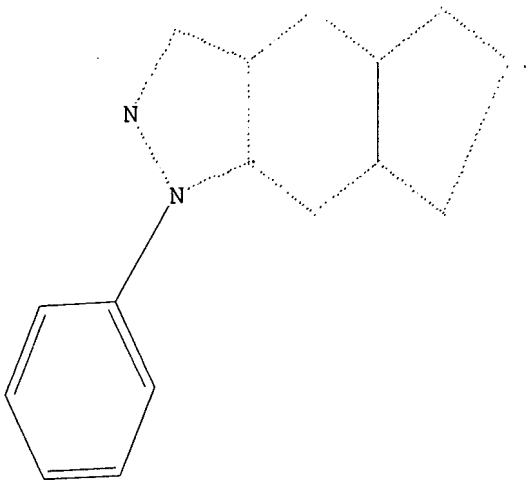

G1 C,N

G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 10:47:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    11557 TO ITERATE

100.0% PROCESSED    11557 ITERATIONS                          273 ANSWERS
SEARCH TIME: 00.00.01

L12          273 SEA SSS FUL L11

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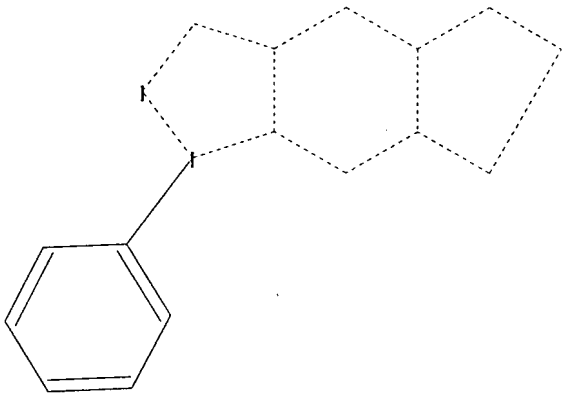

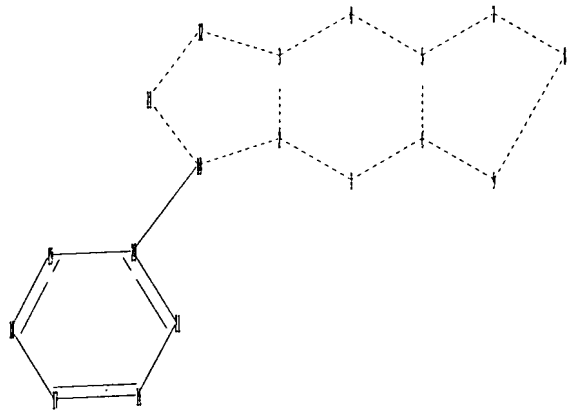

```
ring nodes :
1  2  3  4  5  6  7  8  9  10  11  12  16  17  18  19  20  21
chain bonds :
10-20
ring bonds :
1-2  1-6  2-3  2-10  3-4  3-12  4-5  5-6  5-7  6-9  7-8  8-9  10-11  11-12  16-17  16-21  17-18
 18-19  19-20  20-21
exact/norm bonds :
1-2  1-6  2-3  2-10  3-4  3-12  4-5  5-6  5-7  6-9  7-8  8-9  10-11  10-20  11-12
normalized bonds :
16-17  16-21  17-18  18-19  19-20  20-21
isolated ring systems :
containing 1 :
```

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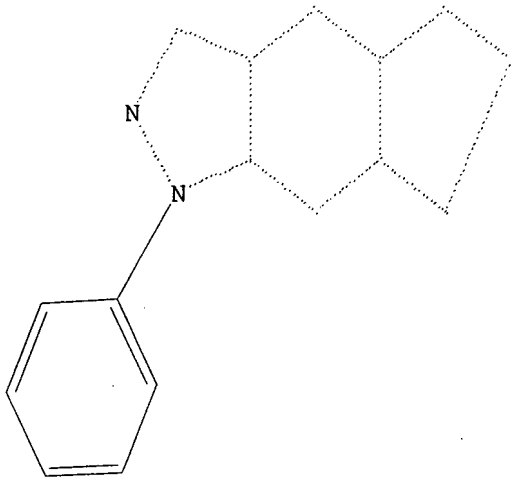
G1:C,N

G2:O,S,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom

L13 STRUCTURE UPLOADED

=> d
L13 HAS NO ANSWERS
L13 STR



G1 C,N
G2 O,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l13 sss sam
SAMPLE SEARCH INITIATED 10:49:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 601 TO ITERATE

100.0% PROCESSED 601 ITERATIONS 14 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 10550 TO 13490
PROJECTED ANSWERS: 56 TO 504

L14 14 SEA SSS SAM L13

=> s l13 sss full
FULL SEARCH INITIATED 10:49:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 11557 TO ITERATE

100.0% PROCESSED 11557 ITERATIONS 277 ANSWERS
SEARCH TIME: 00.00.01

L15 277 SEA SSS FUL L13

=> file hcaplus

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	344.65	739.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.12

FILE 'HCAPLUS' ENTERED AT 10:49:13 ON 26 APR 2007
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FILE COVERS 1907 - 26 Apr 2007 VOL 146 ISS 18
FILE LAST UPDATED: 25 Apr 2007 (20070425/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l15
L16             7 L15

=> s l16 not l5
L17             3 L16 NOT L5

=> d ibib abs hitstr tot
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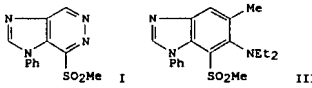
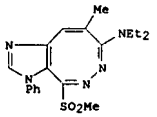
L17 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1991:607969 HCAPLUS
DOCUMENT NUMBER: 115:207969
TITLE: Condensed pyridazines. VIII. Reaction of diazolopyridazines with ynamine. Formation of benzodiazoles and diazolodiazocines
AUTHOR(S): Oishi, Etsuo; Taido, Naokata; Miyashita, Akira; Sato, Susumu; Ohta, Syouji; Ishida, Hitoshi; Tanji, Kenichi; Higashino, Takeo
CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1991), 39(7), 1713-18
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:207969
GI



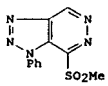
I

III



IV

V

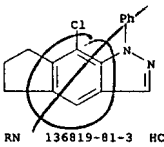


VI

AB Reaction of imidazopyridazine I with MeC.tplbond.CNEt2 (II) resulted in the formation of the benzimidazole III and the 3H-imidazo[4,5-d][1,2]diazocine IV through the [4+2]- and [2+2]cycloadducts. Similarly, reaction of the pyrazolopyridazines V (R = CN, SO2Me) with II gave the corresponding indazoles and pyrazolodiazocines. A similar reaction was also found to proceed between (methylsulfonyl)triazolopyridazines VI and II affording the corresponding benzotriazole and triazolodiazocine.

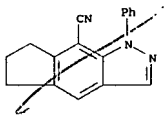
IT 136819-80-2P 136819-81-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 136819-80-2 HCAPLUS
CN Cyclopent[f]indazole, 8-chloro-1,5,6,7-tetrahydro-1-phenyl- (9CI) (CA INDEX NAME)



RN 136819-81-3 HCAPLUS
CN Cyclopent[f]indazole-8-carbonitrile, 1,5,6,7-tetrahydro-1-phenyl- (9CI)

L17 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)

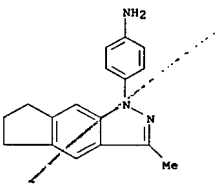


L17 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1968:496557 HCAPLUS
DOCUMENT NUMBER: 69:96557
TITLE: New cyclic systems derived from indazole
AUTHOR(S): Portal, Carlos R.; Dennler, Enrique B.; Frasca, Adolfo R.
CORPORATE SOURCE: Univ. Buenos Aires, Buenos Aires, Argent.
SOURCE: Anales de la Asociacion Quimica Argentina (1967), 55(3-4), 245-51
CODEN: AAQAAE; ISSN: 0365-0375
DOCUMENT TYPE: Journal
LANGUAGE: Spanish
GI For diagram(s), see printed CA Issue.
AB Two new cyclic systems (I and II) were synthesized from the p-nitrophenylhydrazone of 5-acetylindane (III) by cyclization. An equimolar mixture of p-nitrophenylhydrazine and 5-acetylindane in EtOH was heated to precipitate III, m. 188-90° (EtOH). III was treated with 10-15 times its weight of polyphosphoric acid and the mixture heated to 160° 2 min., diluted with water, and extracted with C6H6, the organic phase washed with water, dried, concentrated and chromatographed on an Al2O3 column using C6H6 eluent. The first fraction contained 23% of a mixture of I (R = p-O2NC6H4) (IV) and II (R = p-O2NC6H4) (V). Recrystn. from EtOH yielded IV, m. 189-90°. The recrystn. liquid was evaporated and the residue chromatographed on a silica gel column with petroleum-EtOAc eluent which caused separation into 2 yellow bands. The first band was IV, and the second was V, m. 163-4° (EtOH). IV, 220 mg., was treated with 1 g. SnCl2, 4 ml. concentrate HCl, and 4 ml. AcOH and the mixture refluxed 10 min., cooled, treated with NaOH, and extracted with Et2O, and the ether phase washed with water, and dried to give I (R = p-H2NC6H4) (VI), m. 150-1° (EtOH-water). Similar treatment of V yielded II (R = p-H2NC6H4) (VII), m. 166-7° (EtOH-water). VI (240 mg.) in 11 ml. 25% H2SO4 was treated with 2.4 ml. 10% Na2Cr2O7 and the mixture maintained 2 hrs. at 0°, diluted with water, treated with NaOAc and extracted with Et2O and the extract washed with water, and dried to give I (R = H), m. 203-4° (Et2O-H2O). Similar treatment of V yielded II (R = H), m. 195-6° (EtOH-H2O).

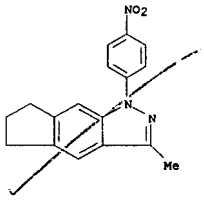
IT 16640-94-1P 16641-17-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectrum (N.M.R. and uv) of)

RN 16640-94-1 HCAPLUS
CN Cyclopent[f]indazole, 1-(p-aminophenyl)-1,5,6,7-tetrahydro-3-methyl- (8CI) (CA INDEX NAME)



RN 16641-17-1 HCAPLUS
CN Cyclopent[f]indazole, 1,5,6,7-tetrahydro-3-methyl-1-(p-nitrophenyl)- (8CI) (CA INDEX NAME)

L17 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



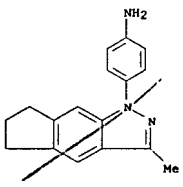
Robert Havlin - 10.544899

L17 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1967:469259 HCAPLUS
DOCUMENT NUMBER: 67:69259
TITLE: The nuclear magnetic resonance spectra of substituted indazoles
AUTHOR(S): Dennler, Enrique B.; Portal, C. R.; Frasca, Adolfo R.
CORPORATE SOURCE: Fac. Cienc. Exact. Nat., Buenos Aires, Argent.
SOURCE: Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy (1967), 23(8), 2243-8
CODEN: SAMCAS; ISSN: 1386-1425
DOCUMENT TYPE: Journal
LANGUAGE: English

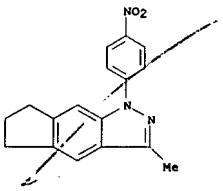
AB Proton magnetic resonance spectra of substituted indazoles, 1-p-aminophenyl-, and 1-p-nitrophenylindazoles are described and the effects of substituents on the pyrazole and benzene rings are discussed.

IT 16640-94-1P 16641-17-1P
RL: PREP (Preparation)
(preparation of)

RN 16640-94-1 HCAPLUS
CN Cyclopent[f]indazole, 1-(p-aminophenyl)-1,5,6,7-tetrahydro-3-methyl- (8CI) (CA INDEX NAME)



RN 16641-17-1 HCAPLUS
CN Cyclopent[f]indazole, 1,5,6,7-tetrahydro-3-methyl-1-(p-nitrophenyl)- (8CI) (CA INDEX NAME)



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=> log hold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	21.01	760.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-5.46

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 10:50:08 ON 26 APR 2007

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Welcome to STN International! Enter x:x

LOGINID:SSPTARHH1626

PASSWORD:
* * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'HCAPLUS' AT 10:56:07 ON 26 APR 2007
FILE 'HCAPLUS' ENTERED AT 10:56:07 ON 26 APR 2007
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	21.01	760.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-5.46

=> file hcaplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	21.01	760.65

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.34	-5.46

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FILE COVERS 1907 - 26 Apr 2007 VOL 146 ISS 18
FILE LAST UPDATED: 25 Apr 2007 (20070425/ED)

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=> s us200!-544899/apps
4 US200!-544899/AP
0 US200!-544899/PRN
L18 4 US200!-544899/APPS
(US200!-544899/AP,PRN)

=> d ibib

L18 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:1005939 HCAPLUS
DOCUMENT NUMBER: 143:294198
TITLE: Electrochemical fabrication process including process monitoring, making corrective action decisions, and taking appropriate actions
INVENTOR(S): Cohen, Adam L.; Lockard, Michael S.; Smalley, Dennis R.; Kilgo, Marvin M.
PATENT ASSIGNEE(S): Microfabrica Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 28 pp., Cont.-in-part of U.S. Ser. No. 434,494.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 37
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005202660	A1	20050915	US 2004-995609	20041122
EP 1518822	A2	20050330	EP 2004-15983	20021206
EP 1518822	A3	20070228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2004000489	A1	20040101	US 2003-434494	20030507
US 2004007470	A1	20040115	US 2003-434519	20030507
AU 2003280468	A1	20040119	AU 2003-280468	20030627
US 2007045122	A1	20070301	US 2006-544899	20061006 <--

PRIORITY APPLN. INFO.:

US 2002-379130P	P	20020507
US 2002-379132P	P	20020507
US 2003-434494	A2	20030507
US 2003-434519	A2	20030507
US 2001-340372P	P	20011206
US 2002-364261P	P	20020313
US 2002-379133P	P	20020507
US 2002-379135P	P	20020507
US 2002-379177P	P	20020507
US 2002-379182P	P	20020507
US 2002-379184P	P	20020507
US 2002-392531P	P	20020627
US 2002-415371P	P	20021001
US 2002-415374P	P	20021001
US 2002-422007P	P	20021029
US 2002-422982P	P	20021101
US 2002-429483P	P	20021126
US 2002-429484P	P	20021126
US 2002-309521	A	20021203
US 2002-430809P	P	20021203
EP 2002-786937	A3	20021206
US 2003-464504P	P	20030421
US 2003-434103	A	20030507
US 2003-434295	A	20030507
US 2003-434497	A	20030507
US 2003-476554P	P	20030606
WO 2003-US20458	W	20030627

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=> d ibib 2

L18 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:303040 HCAPLUS
DOCUMENT NUMBER: 142:344105
TITLE: Multi-step release method for electrochemically fabricated structures
INVENTOR(S): Cohen, Adam L.; Lockard, Michael S.; McPherson, Dale S.
PATENT ASSIGNEE(S): Microfabrica Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 32 pp., Cont.-in-part of U.S. Ser. No. 607,931.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 37
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005072681	A1	20050407	US 2004-841347	20040507
US 2003222738	A1	20031204	US 2002-309521	20021203
EP 1518822	A2	20050330	EP 2004-15983	20021206
EP 1518822	A3	20070228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2004004001	A1	20040108	US 2003-434295	20030507
US 2004007468	A1	20040115	US 2003-434497	20030507
US 2004007470	A1	20040115	US 2003-434519	20030507
US 2004020782	A1	20040205	US 2003-434103	20030507
US 7160429	B2	20070109		
WO 2004004061	A1	20040108	WO 2003-US20458	20030627
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AU 2003280468	A1	20040119	AU 2003-280468	20030627
CN 1669177	A	20050914	CN 2003-817237	20030627
WO 2004032210	A2	20040415	WO 2003-US31244	20031001
WO 2004032210	A3	20050609		
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AU 2003279763	A1	20040423	AU 2003-279763	20031001
TW 236453	B	20050721	TW 2003-92132582	20031120
TW 244799	B	20051201	TW 2004-93116127	20040604
US 2005221529	A1	20051006	US 2005-139391	20050527
US 2007045122	A1	20070301	US 2006-544899	20061006 <--

PRIORITY APPLN. INFO.:

US 2001-338638P	P	20011203
US 2001-340372P	P	20011206
US 2002-379130P	P	20020507
US 2002-379133P	P	20020507

L18 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

US 2002-379182P	P	20020507
US 2002-379184P	P	20020507
US 2002-392531P	P	20020627
US 2002-415374P	P	20021001
US 2002-309521	A2	20021203
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US 2003-464504P	P	20030421
US 2003-434103	A2	20030507
US 2003-434295	A2	20030507
US 2003-434497	A2	20030507
US 2003-434519	A2	20030507
US 2003-476554P	P	20030606
US 2003-607931	A2	20030627
US 2002-364261P	P	20020313
US 2002-379135P	P	20020507
US 2002-379177P	P	20020507
US 2002-415371P	P	20021001
US 2002-422007P	P	20021029
US 2002-422982P	P	20021101
US 2002-429483P	P	20021126
US 2002-429484P	P	20021126
EP 2002-786937	A3	20021206
US 2002-313795	A1	20021206
WO 2003-US20458	W	20030627
WO 2003-US31244	W	20031001

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=> d ibib 3

L18 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:98637 HCAPLUS
DOCUMENT NUMBER: 142:187861
TITLE: Methods for electrochemically fabricating multi-layer structures including regions incorporating maskless, patterned, multiple layer thickness depositions of selected materials
INVENTOR(S): Cohen, Adam L.; Smalley, Dennis R.
PATENT ASSIGNEE(S): Microfabrica Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 35 pp., Cont.-in-part of U.S. Ser. No. 434,519.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 37
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005023144	A1	20050203	US 2004-841001	20040507
EP 1518822	A2	20050330	EP 2004-15983	20021206
EP 1518822	A3	20070228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, MK, CY, AL, TR, BG, CZ, EE, SK				
US 2004007470	A1	20040115	US 2003-434519	20030507
AU 2003280468	A1	20040119	AU 2003-280468	20030627
US 2007045122	A1	20070301	US 2006-544899	20061006 <--

PRIORITY APPLN. INFO.:

US 2002-379130P	P	20020507
US 2003-434519	A2	20030507
US 2003-468908P	P	20030507
US 2001-340372P	P	20011206
US 2002-364261P	P	20020313
US 2002-379133P	P	20020507
US 2002-379135P	P	20020507
US 2002-379177P	P	20020507
US 2002-379182P	P	20020507
US 2002-379184P	P	20020507
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US 2002-415371P	P	20021001
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US 2002-309521	A	20021203
US 2002-430809P	P	20021203
EP 2002-786937	A3	20021206
US 2003-464504P	P	20030421
US 2003-434103	A	20030507
US 2003-434295	A	20030507
US 2003-434497	A	20030507
US 2003-476554P	P	20030606
WO 2003-US20458	W	20030627

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=> d ibib 4

L18 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:740124 HCAPLUS
DOCUMENT NUMBER: 141:260743
TITLE: Preparation of cyclopent[f]indazole and benz[f]indazole derivatives selective non-steroidal glucocorticoid receptor modulators
INVENTOR(S): Ali, Amjad; Beresis, Richard; Colletti, Steven L.; Graham, Donald W.; Tata, James R.; Thompson, Christopher F.
PATENT ASSIGNEE(S): Merck & Co. Inc., USA
SOURCE: PCT Int. Appl., 105 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004075840	A2	20040910	WO 2004-US5199		20040220
WO 2004075840	A3	20050203			
WO 2004075840	A9	20050804			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2004216182	A1	20040910	AU 2004-216182		20040220
CA 2516684	A1	20040910	CA 2004-2516684		20040220
EP 1599201	A2	20051130	EP 2004-713398		20040220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2006518752	T	20060817	JP 2006-503780		20040220
US 2006074120	A1	20060406	US 2005-544899		20050808 <--
PRIORITY APPLN. INFO.:			US 2003-450811P	P	20030225
			WO 2004-US5199	W	20040220

OTHER SOURCE(S): MARPAT 141:260743

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=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	9.92	770.57

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.46

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DICTIONARY FILE UPDATES: 25 APR 2007 HIGHEST RN 932710-95-7

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experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

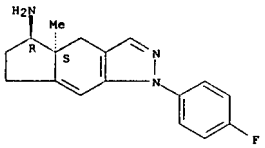
http://www.cas.org/support/stngen/stndoc/properties.html

=> tra rn l18 4
L19 TRANSFER L18 4 RN : 282 TERMS
L20 282 L19

=> d scan

L20 282 ANSWERS REGISTRY COPYRIGHT 2007 ACS on STN
IN Cyclopent[f]indazol-5-amine, 1-(4-fluorophenyl)-1,4,4a,5,6,7-hexahydro-4a-methyl-, (4aS,5R)- (9CI)
MF C17 H18 F N3

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

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=> file hcaplus
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.45	785.27

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.46

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FILE COVERS 1907 - 26 Apr 2007 VOL 146 ISS 18
FILE LAST UPDATED: 25 Apr 2007 (20070425/ED)

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substance identification.

=> s l20
L21 408632 L20

=> file reg
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.60	787.87

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-5.46

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STRUCTURE FILE UPDATES: 25 APR 2007 HIGHEST RN 932710-95-7
DICTIONARY FILE UPDATES: 25 APR 2007 HIGHEST RN 932710-95-7

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TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

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http://www.cas.org/support/stngen/stndoc/properties.html

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      18452292 N>=2
       3718411 F>=1
L22         262 L20 AND C>=16 AND N>=2 AND F>=1

=> file hcaplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                      15.75     803.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -5.46

FILE 'HCAPLUS' ENTERED AT 10:58:52 ON 26 APR 2007
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FILE LAST UPDATED: 25 Apr 2007  (20070425/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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L23           7 L22

=> d hist

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L1              STRUCTURE UPLOADED
L2           14 S L1 SSS SAM

     FILE 'HCAPLUS' ENTERED AT 10:28:33 ON 26 APR 2007
L3            3 S L2

     FILE 'REGISTRY' ENTERED AT 10:32:56 ON 26 APR 2007
L4          272 S L1 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 10:33:15 ON 26 APR 2007
L5            4 S L4
L6            1 S L5 NOT L3

     FILE 'REGISTRY' ENTERED AT 10:45:22 ON 26 APR 2007
L7              STRUCTURE UPLOADED
L8          194 S L7 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 10:46:02 ON 26 APR 2007
L9            4 S L8
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L10           0 S L9 NOT L5

     FILE 'REGISTRY' ENTERED AT 10:47:24 ON 26 APR 2007
L11               STRUCTURE UPLOADED
L12           273 S L11 SSS FULL
L13               STRUCTURE UPLOADED
L14            14 S L13 SSS SAM
L15           277 S L13 SSS FULL

     FILE 'HCAPLUS' ENTERED AT 10:49:13 ON 26 APR 2007
L16             7 S L15
L17             3 S L16 NOT L5

     FILE 'HCAPLUS' ENTERED AT 10:56:14 ON 26 APR 2007
L18             4 S US200!-544899/APPS

     FILE 'REGISTRY' ENTERED AT 10:57:13 ON 26 APR 2007

     FILE 'HCAPLUS' ENTERED AT 10:57:22 ON 26 APR 2007
L19               TRA L18 4 RN :      282 TERMS

     FILE 'REGISTRY' ENTERED AT 10:57:23 ON 26 APR 2007
L20           282 SEA L19

     FILE 'HCAPLUS' ENTERED AT 10:57:38 ON 26 APR 2007
L21        408632 S L20

     FILE 'REGISTRY' ENTERED AT 10:57:50 ON 26 APR 2007
L22           262 S L20 AND C>=16 AND N>=2 AND F>=1

     FILE 'HCAPLUS' ENTERED AT 10:58:52 ON 26 APR 2007
L23             7 S L22

=> s l23 not l16
L24             3 L23 NOT L16

=> d ibib abs hitstr tot
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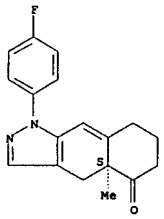
L24 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:767304 HCAPLUS
DOCUMENT NUMBER: 141:405644
TITLE: Design and evaluation of novel nonsteroidal dissociating glucocorticoid receptor ligands
AUTHOR(S): Shah, Nilesh; Scanlan, Thomas S.
CORPORATE SOURCE: Graduate Group in Biophysics, University of California, San Francisco, CA, 94143-2280, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(20), 5199-5203
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:405644

AB A novel class of phenylpyrazole fused Wieland-Miescher ketone derivs. are high affinity, receptor specific, selective modulators of glucocorticoid receptor (GR) mediated transcription in vitro, dissociating transactivation, AP-1 repression, and NF-κB repression from each other.

IT 614763-00-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(design and evaluation of novel nonsteroidal dissociating glucocorticoid receptor ligands)

RN 614763-00-7 HCAPLUS
CN 5H-Benz[f]indazol-5-one, 1-(4-fluorophenyl)-1,4,4a,6,7,8-hexahydro-4a-methyl-, (4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

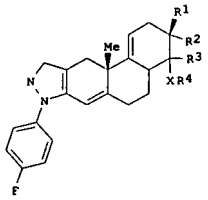


REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

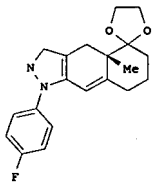
L24 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:270010 HCAPLUS
DOCUMENT NUMBER: 140:287380
TITLE: Preparation of octahydro-2-H-naphtho[1,2-f]indole-4-carboxamide derivatives as selective glucocorticoid receptor modulators for the treatment of autoimmune and inflammatory conditions
INVENTOR(S): Ali, Amjad; Aster, Susan D.; Balkovec, James M.; Graham, Donald W.; Hunt, Julianne A.; Kallashi, Florida; Sinclair, Peter J.; Tata, James R.; Taylor, Gayle E.; Goulet, Joung L.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026248	A2	20040401	WO 2003-US29494	20030917
WO 2004026248	A3	20040715		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2499150	A1	20040401	CA 2003-2499150	20030917
AU 2003270783	A1	20040408	AU 2003-270783	20030917
EP 1542996	A2	20050622	EP 2003-752495	20030917
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006503107	T	20060126	JP 2004-568945	20030917
US 2005245588	A1	20051103	US 2005-527615	20050311
PRIORITY APPLN. INFO.:			US 2002-412231P P	20020920
			US 2003-476079P P	20030605
			WO 2003-US29494 W	20030917

OTHER SOURCE(S): MARPAT 140:287380
GI



I



II

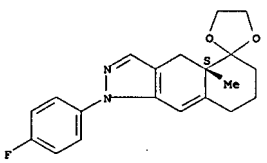
L24 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Octahydro-2-H-naphtho[1,2-f]indole-4-carboxamide derivs. I (X = CO, NHCO, CONH, NH, CH2NH; R1,R2 = H, alkyl, alkenyl, cycloalkyl, alkoxy, aryl; R3 = alkyl, alkoxy, acid, halogen substituted alkyl; R4 = alkyl, alkenyl, cycloalkoxy, alkoxy, aryl) were prepared as selective glucocorticoid receptor modulators for the treatment of autoimmune and inflammatory conditions. Thus, (S)-Wieland-Miescher ketone was protected as the ketal using p-toluene sulfonic acid and ethylene glycol and then treated with Et formate to give the hydroxymethylene ketal derivative The hydroxymethylene was dissolved in acetic acid and reacted with p-fluorophenyl hydrazine hydrochloride to give II. The ketal of II was converted to the ketone using 6N HCl, and the resulting ketone transformed into the triflate. The triflate was treated with tributylvinyl tin and PPh3 to give the corresponding coupling product. Treatment with ethyl-4,4,4-trifluorocrotonate followed by dropwise addition of BCl3 gave the target I (R1 = CF3, R2, R3 = H, X = CO, R4 = OEt),.

IT 614762-99-1P 614763-00-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of octahydronaphthoindole-4-carboxamide derivs. as selective glucocorticoid receptor modulators for the treatment of autoimmune and inflammatory conditions)

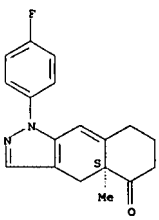
RN 614762-99-1 HCAPLUS
CN Spiro[5H-benz[f]indazole-5,2'-[1,3]dioxolane], 1-(4-fluorophenyl)-1,4,4a,6,7,8-hexahydro-4a-methyl-, (4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

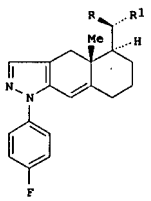


RN 614763-00-7 HCAPLUS
CN 5H-Benz[f]indazol-5-one, 1-(4-fluorophenyl)-1,4,4a,6,7,8-hexahydro-4a-methyl-, (4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:267662 HCAPLUS
DOCUMENT NUMBER: 141:7063
TITLE: Novel N-Arylpyrazolo[3,2-c]-Based Ligands for the Glucocorticoid Receptor: Receptor Binding and in Vivo Activity
AUTHOR(S): Ali, Amjad; Thompson, Christopher F.; Balkovec, James M.; Graham, Donald W.; Hammond, Milton L.; Quraishi, Nazia; Tata, James R.; Einstein, Monica; Ge, Lan; Harris, Georgianna; Kelly, Terri M.; Mazur, Paul; Pandit, Shilpa; Santoro, Joseph; Sitlani, Ayesha; Wang, Chuanlin; Williamson, Joanne; Miller, Douglas K.; Thompson, Chris M.; Zaller, Dennis M.; Forrest, Michael J.; Carballo-Jane, Ester; Luell, Silvi
CORPORATE SOURCE: Departments of Medicinal Chemistry, Metabolic Disorders Immunonology and Pharmacology, Merck Research Laboratories, Rahway, NJ, 07065, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(10), 2441-2452
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:7063
GI



I

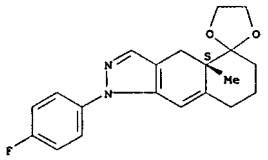
AB A novel series of selective ligands for the human glucocorticoid receptor (hGR) are described. Preliminary structure-activity relationships were focused on substitution at C-1 and indicated a preference for 3-, 4-, and 5-substituted aromatic and benzylic groups. The resulting analogs, e.g., I [R = OH, R1 = 3,4,5-MeO(F2)C6H2, CH2C6H4F-4], exhibited excellent affinity for hGR (IC50 1.9 nM and 2.8 nM, resp.) and an interesting partial agonist profile in functional assays of transactivation (tyrosine aminotransferase, TAT, and glutamine synthetase, GS) and transrepression (IL-6). The most potent compds. were I [R = 4-FC6H4, 2-thienyl, R1 = OH]. These candidates showed highly efficacious IL-6 inhibition vs. dexamethasone. I [R = 2-thienyl, R1 = OH] was evaluated in vivo in the mouse LPS challenge model and showed an ED50 = 4.0 mg/kg, compared to 0.5 mg/kg for prednisolone in the same assay.

IT 614762-99-1P 614763-00-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and glucocorticoid receptor binding of [aryl(hydroxy)methyl]naphthopyrazoles)

RN 614762-99-1 HCAPLUS
CN Spiro[5H-benz[f]indazole-5,2'-[1,3]dioxolane], 1-(4-fluorophenyl)-1,4,4a,6,7,8-hexahydro-4a-methyl-, (4aS)- (9CI) (CA INDEX NAME)

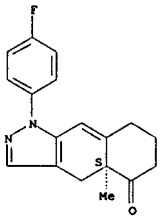
Absolute stereochemistry.

L24 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 614763-00-7 HCAPLUS
CN 5H-Benz[f]indazol-5-one, 1-(4-fluorophenyl)-1,4,4a,6,7,8-hexahydro-4a-methyl-, (4aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT